

# Bayesian large-scale structure inference

Likelihood-based and likelihood-free approaches

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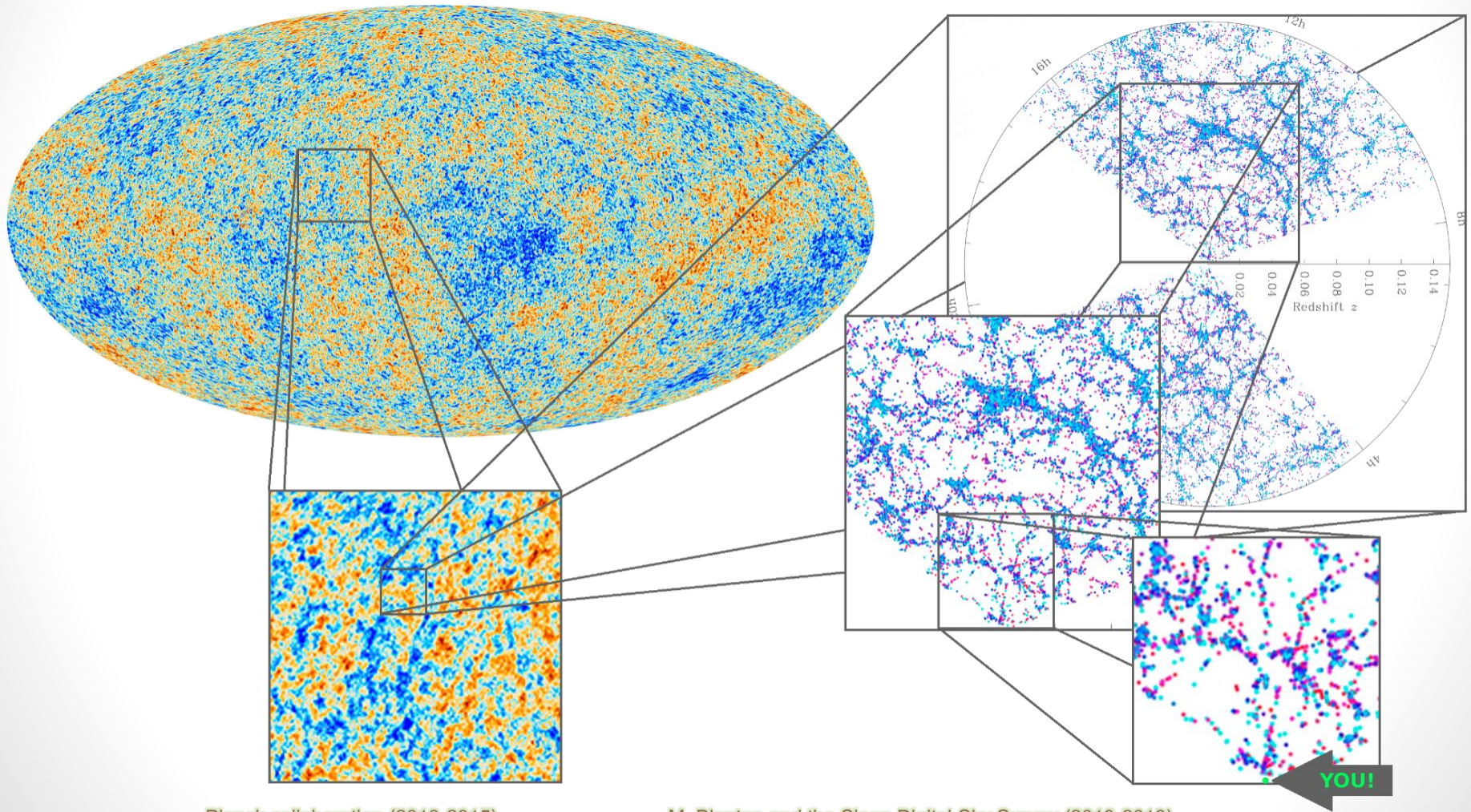
In collaboration with:

Wolfgang Enzi (MPA), Jens Jasche (ExC Garching/U.  
Stockholm), Guilhem Lavaux (IAP),  
Will Percival (U. Portsmouth), Benjamin Wandelt (IAP/CCA)



# The big picture: the Universe is highly structured

*You are here. Make the best of it...*



Planck collaboration (2013-2015)

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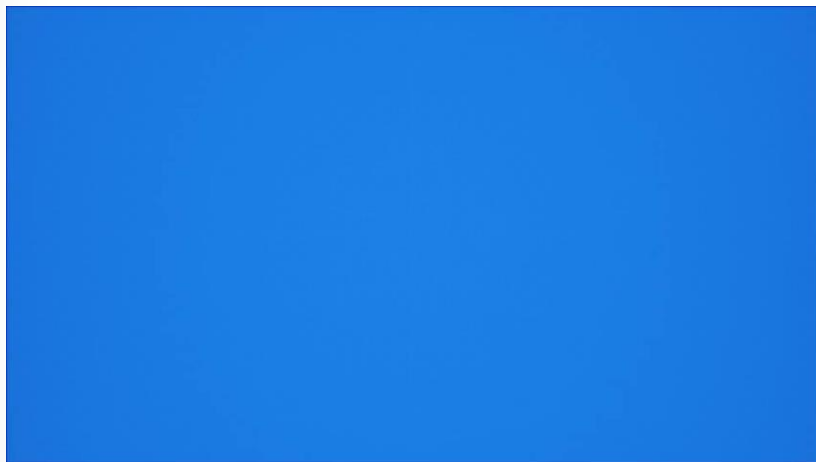
M. Blanton and the Sloan Digital Sky Survey (2010-2013)

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# What we want to know from the LSS

The LSS is a vast source of knowledge:

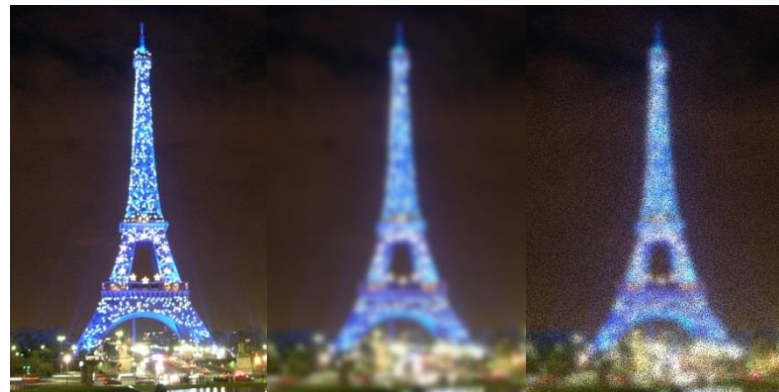
- **Cosmology:**
  - Cosmological parameters and tests of  $\Lambda$ CDM,
  - Physical nature of the dark components,
  - Geometry of the Universe,
  - Tests of General Relativity,
  - Initial conditions and link to high energy physics
- **Astrophysics:** galaxy formation and evolution as a function of their environment
  - Galaxy properties (colours, chemical composition, shapes),
  - Intrinsic alignments



Y. Dubois & S. Colombi (IAP)

# Why Bayesian inference?

- Inference of signals = ill-posed problem
  - Incomplete observations: finite resolution, survey geometry, selection effects
  - Noise, biases, systematic effects
  - Cosmic variance



➡ No unique recovery is possible!

“What is the formation history of the Universe?”



“What is the probability distribution of possible formation histories (signals) compatible with the observations?”

**Bayes' theorem:**  $\mathcal{P}(s|d)\mathcal{P}(d) = \mathcal{P}(d|s)\mathcal{P}(s)$

- Cox-Jaynes theorem: Any system to manipulate “*plausibilities*”, consistent with Cox’s desiderata, is isomorphic to **(Bayesian) probability theory**

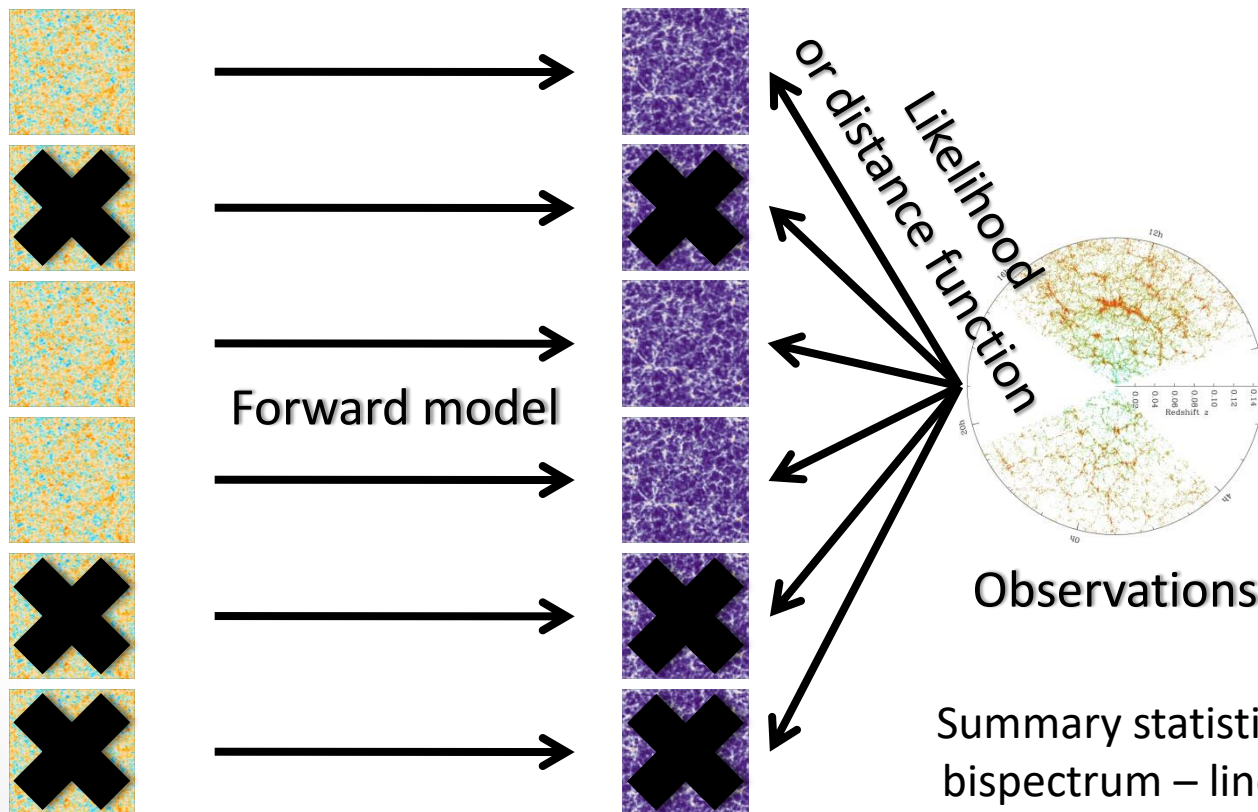


How to do that?

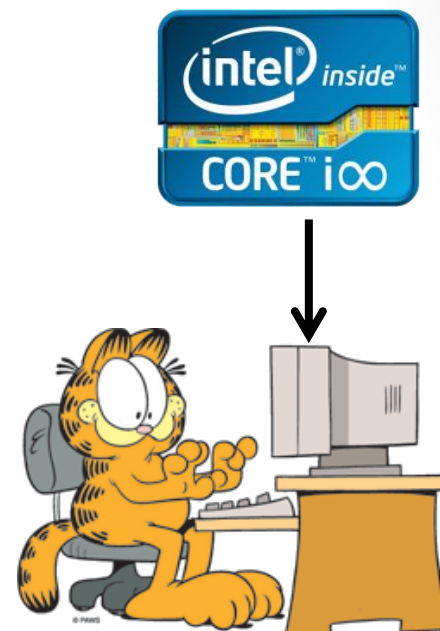


# Bayesian forward modeling: the ideal scenario

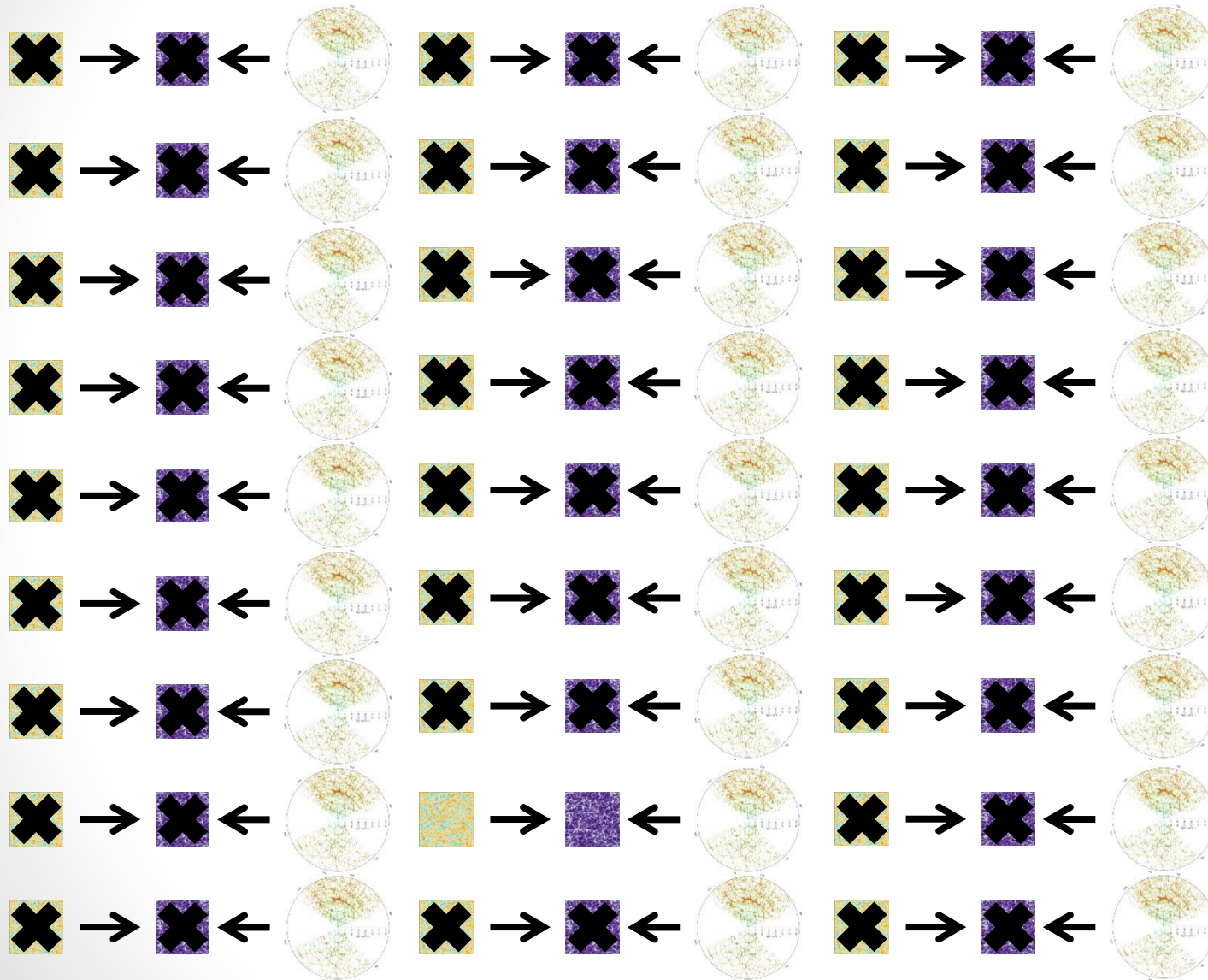
Forward model = N-body simulation + Halo occupation +  
Galaxy formation + Feedback + ...



Summary statistic = power spectrum –  
bispectrum – line correlation function  
– clusters – voids...



# Bayesian forward modeling: the challenge



$d \approx 10^7$

# LIKELIHOOD-BASED SOLUTION: BORG

Exact statistical inference  
Approximate physical model



# Hamiltonian (Hybrid) Monte Carlo

- Use classical mechanics to solve statistical problems!

- The potential:  $\psi(\mathbf{x}) \equiv -\ln p(\mathbf{x})$

- The Hamiltonian:  $H(\mathbf{x}, \mathbf{p}) \equiv \frac{1}{2} \mathbf{p}^\top \mathbf{M}^{-1} \mathbf{p} + \psi(\mathbf{x})$

$$(\mathbf{x}, \mathbf{p}) \Rightarrow \left\{ \begin{array}{l} \frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}} = \mathbf{M}^{-1} \mathbf{p} \\ \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} = -\frac{d\psi(\mathbf{x})}{d\mathbf{x}} \end{array} \right\} \Rightarrow (\mathbf{x}', \mathbf{p}')$$

gradients of the pdf

$$a(\mathbf{x}', \mathbf{x}) = e^{-(H' - H)} = 1 \leftarrow \text{acceptance ratio unity}$$

- HMC **beats the curse of dimensionality** by:

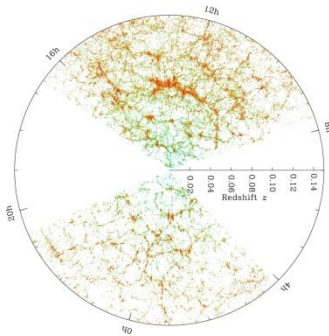
- Exploiting gradients
- Using conservation of the Hamiltonian



# BORG: *Bayesian Origin Reconstruction from Galaxies*

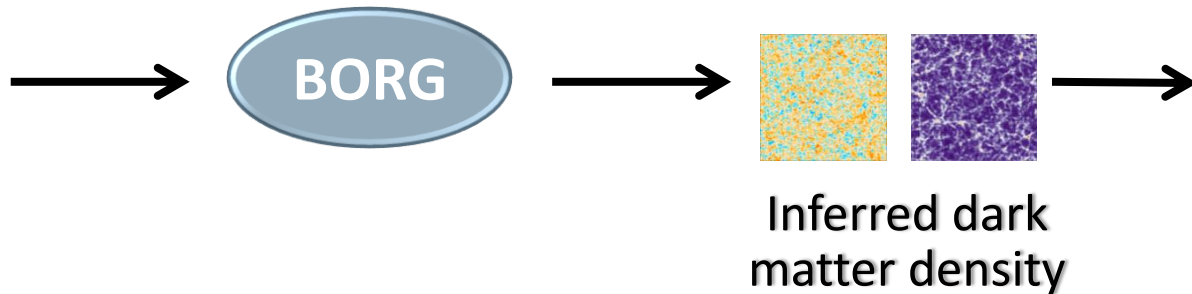


- **Sampler:** Hamiltonian Monte Carlo
- **Data model:**
  - Gaussian prior for the initial conditions
  - Second-order Lagrangian perturbation theory (2LPT)
  - Poisson likelihood



Observations

(galaxy catalog + meta-data: selection functions, completeness...)



Inferred dark matter density

Cosmic web analysis

see also:

Kitaura 2013, arXiv:1203.4184

Wang, Mo, Yang & van den Bosch 2013, arXiv:1301.1348

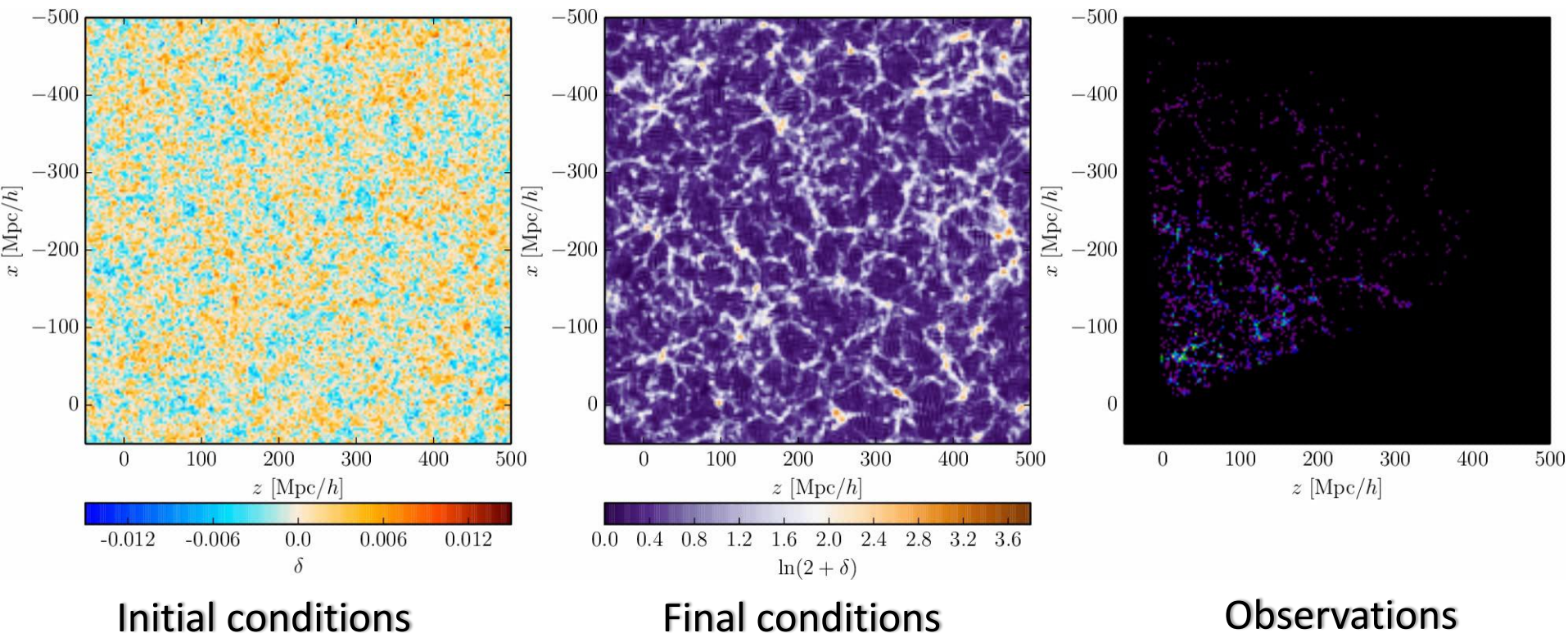
Jasche & Wandelt 2013, arXiv:1203.3639

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# Likelihood-based solution: BORG at work

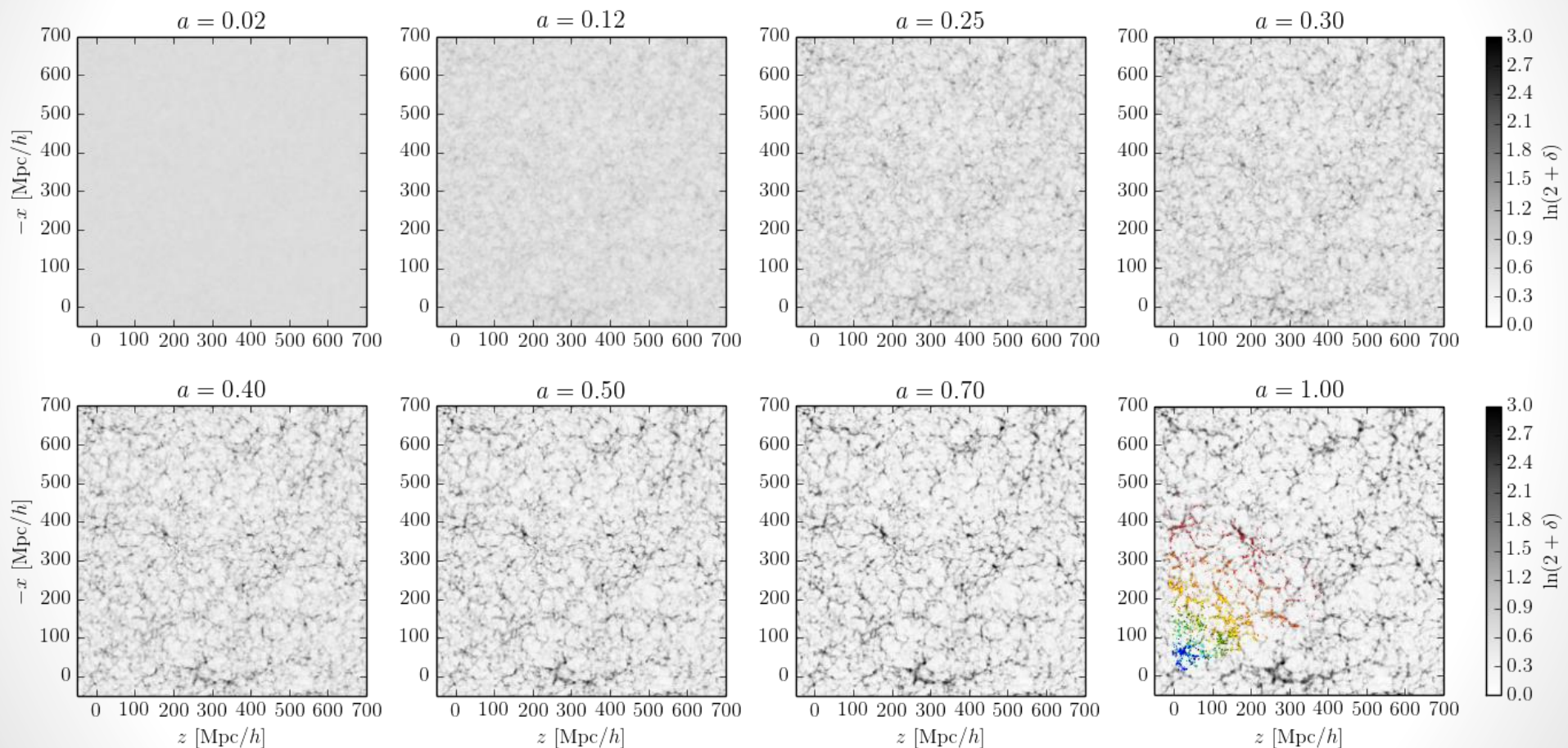
uses Hamiltonian Monte Carlo (HMC) to explore the exact posterior



334,074 galaxies,  $\approx 17$  millions parameters, 3 TB of primary data products,  
12,000 samples,  $\approx 250,000$  data model evaluations, 10 months on 32 cores

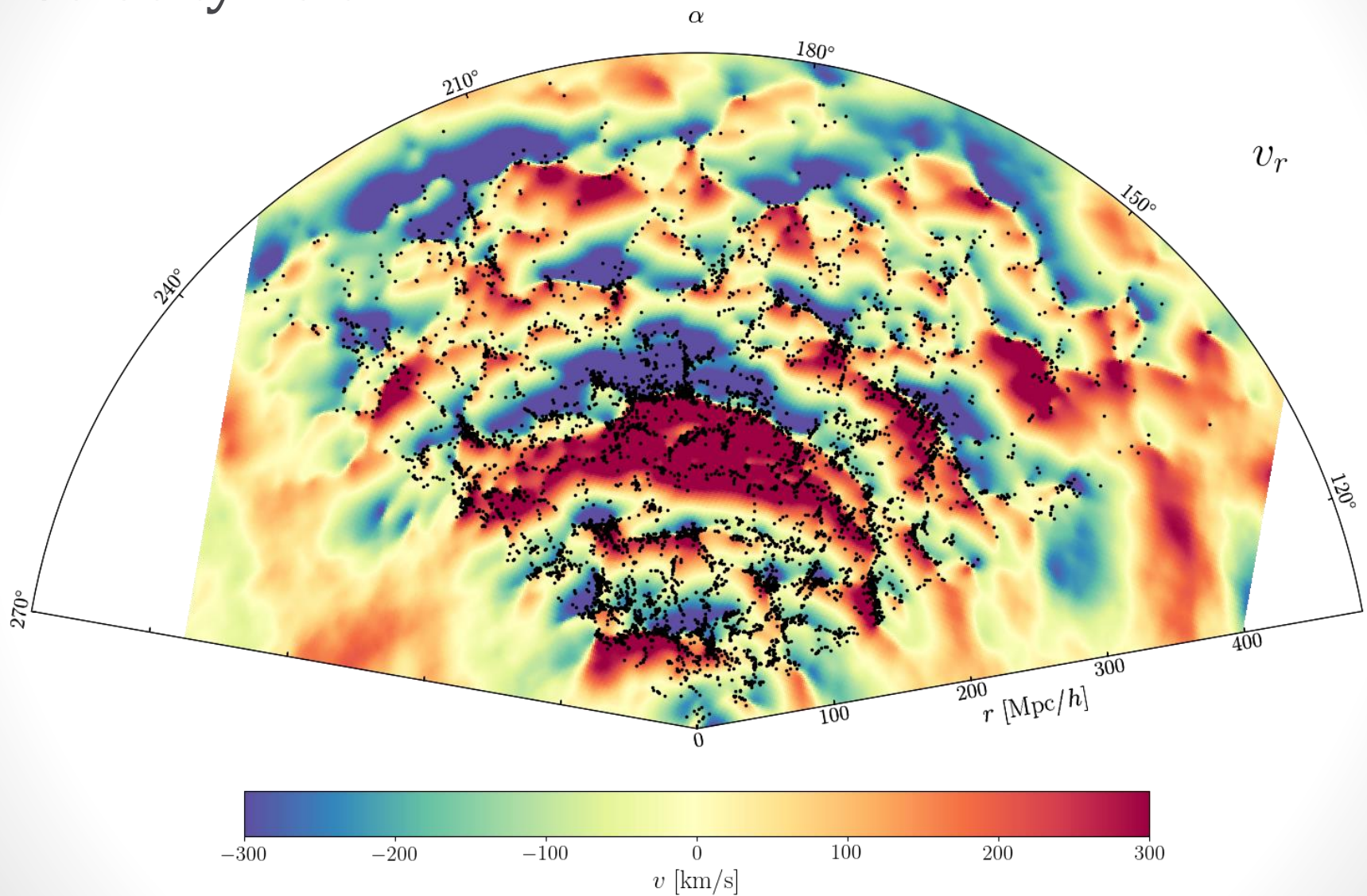
Jasche, FL & Wandelt 2015, arXiv:1409.6308

# Evolution of cosmic structure



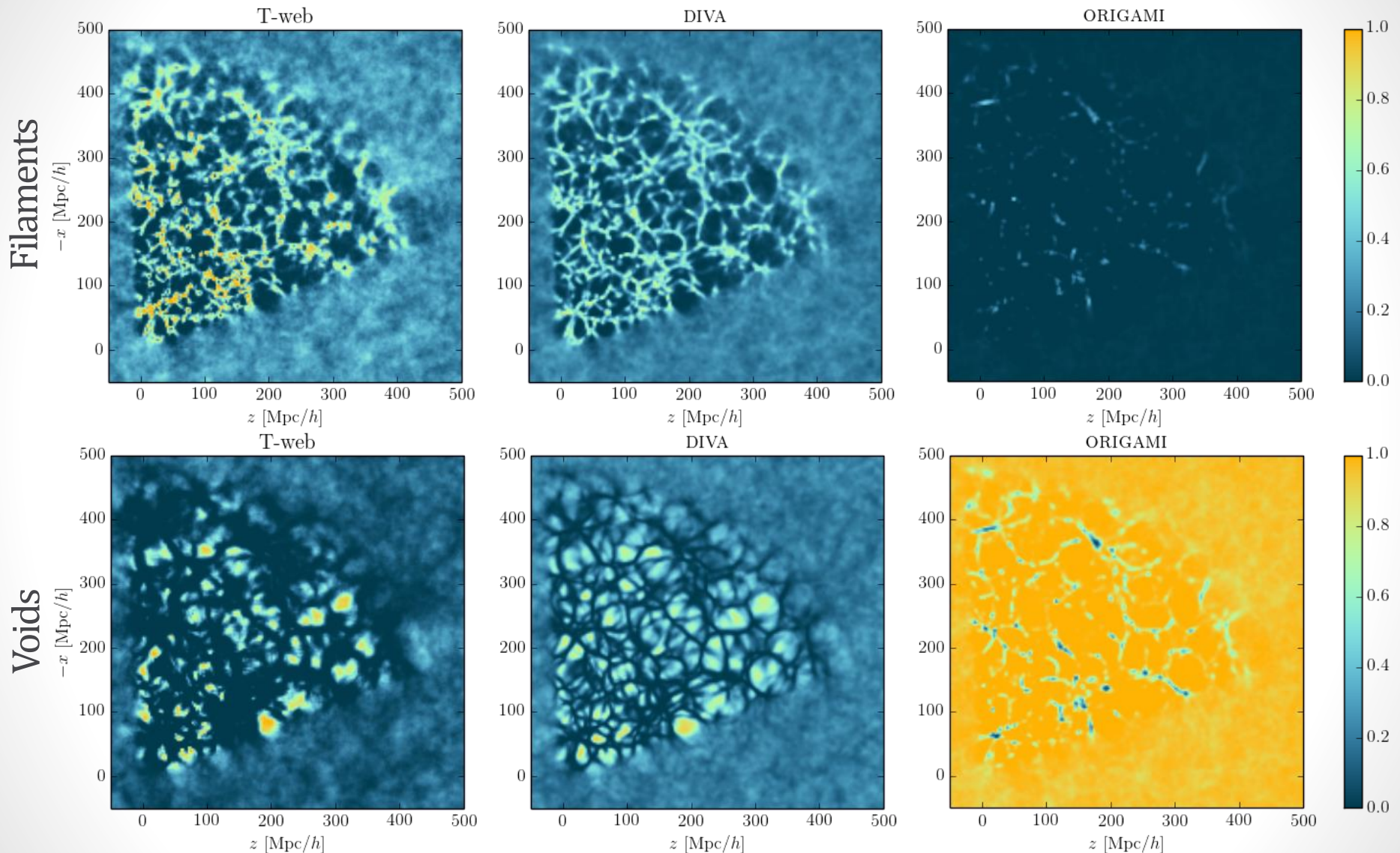


# Velocity field



FL, Jasche, Lavaux, Wandelt & Percival 2017, arXiv:1601.00093

# Cosmic web classifications



FL, Jasche & Wandelt 2015a, arXiv:1502.02690

FL, Lavaux, Jasche & Wandelt 2016, arXiv:1606.06758

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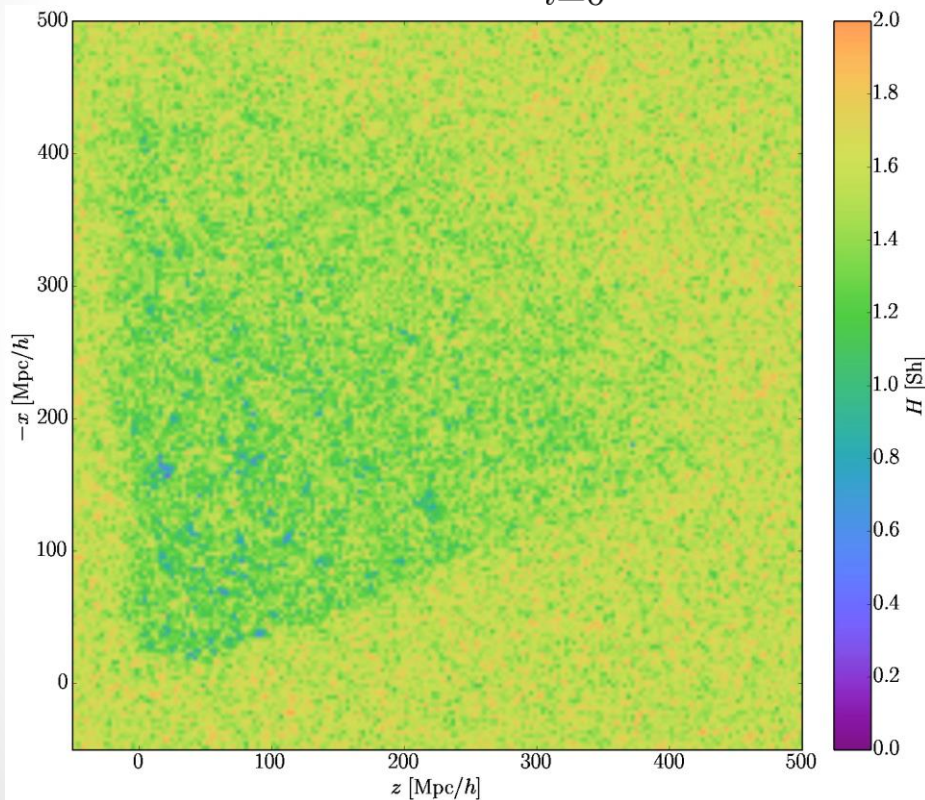
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# How is information propagated?

Shannon entropy

$$H [\mathcal{P}(\mathbf{T}(\vec{x}_k)|d)] \equiv - \sum_{i=0}^3 \mathcal{P}(\mathbf{T}_i(\vec{x}_k)|d) \log_2(\mathcal{P}(\mathbf{T}_i(\vec{x}_k)|d)) \quad \text{in shannons (Sh)}$$



More about cosmic web analysis:

FL, Jasche & Wandelt 2015a, arXiv:1502.02690

(T-web, entropy, relative entropy)

FL, Jasche & Wandelt 2015b, arXiv:1503.00730

(decision theory for structure classification)

FL, Lavaux, Jasche & Wandelt 2016, arXiv:1606.06758

(mutual information, classifier utilities)

FL, Jasche, Lavaux, Wandelt & Percival 2017

(phase-space structure of dark matter)

# INTERLUDE

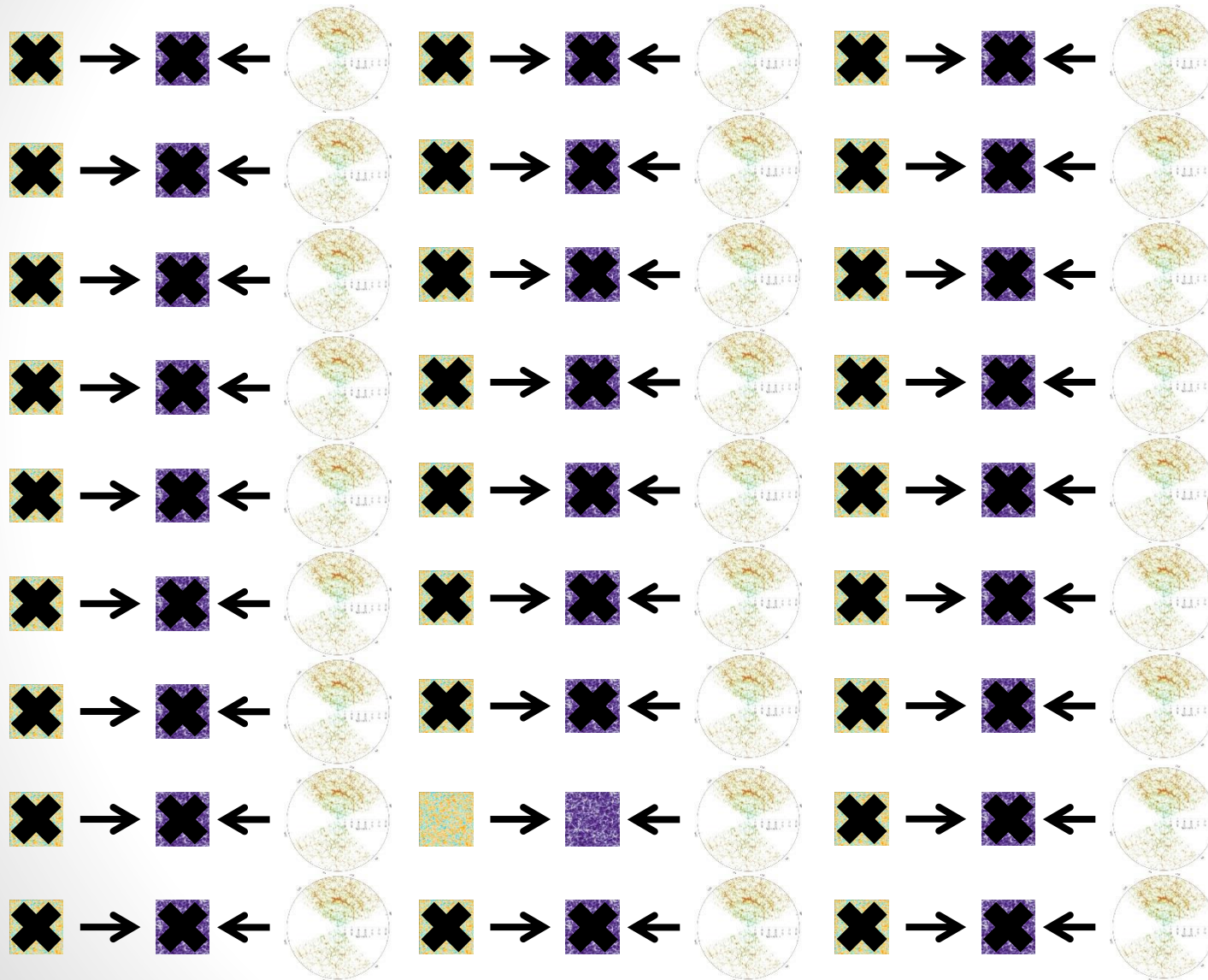
# Mapping the Universe: epilogue?



J. Cham – PhD comics



# Let's go back to the challenge...



$d \approx 10^7$



# LIKELIHOOD-FREE SOLUTION: BOLFI



Approximate statistical inference  
Exact physical model



# Approximate Bayesian Computation (ABC)

- Statistical inference for models where:
  1. The likelihood function is intractable
  2. Simulating data is possible
- **General idea:** find parameter values for which the distance between simulated data and observed data is small

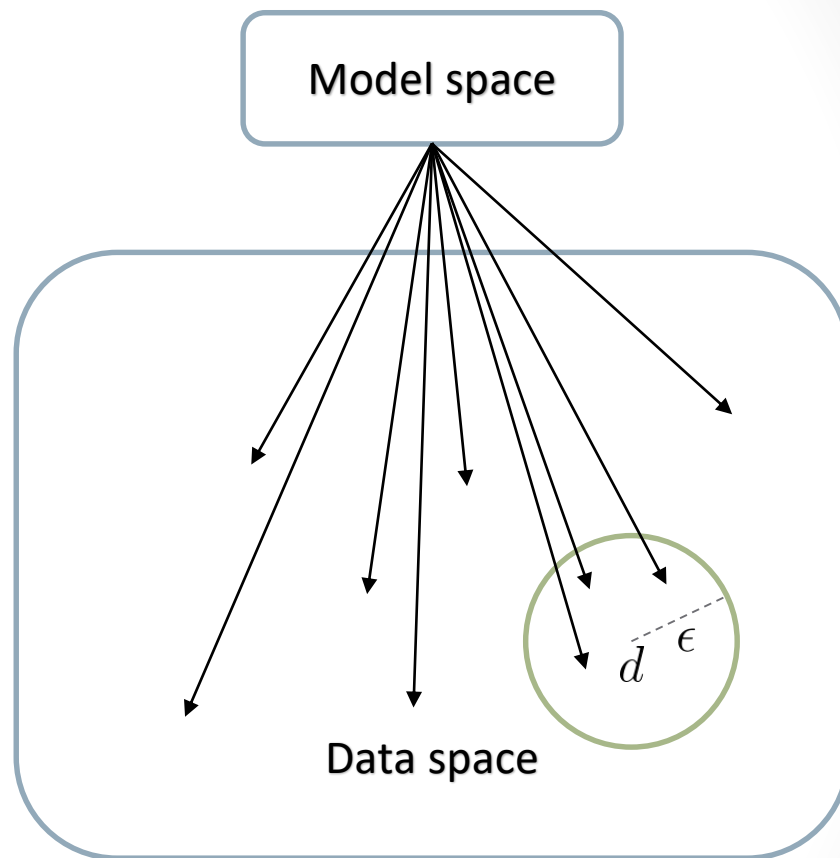
$$p(\theta|d) \Rightarrow p(\theta|\tilde{d}) \quad \text{where } d(\tilde{d}(\theta), d) \text{ is small}$$

- **Assumptions:**
  - Only a small number of parameters are of interest
  - But the process generating the data is very general: a noisy non-linear dynamical system with an unrestricted number of hidden variables

# Likelihood-free rejection sampling

- Iterate many times:
  - Sample  $\theta$  from a proposal distribution  $q(\theta)$
  - Simulate  $\tilde{d}(\theta)$  according to the data model
  - Compute distance  $d(\tilde{d}(\theta), d)$  between simulated and observed data
  - Retain  $\theta$  if  $d(\tilde{d}(\theta), d) \leq \epsilon$ , otherwise reject
- Effective likelihood approximation:

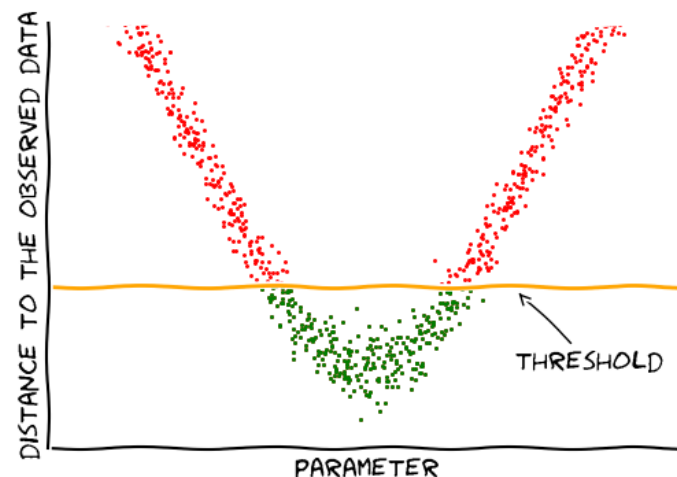
$$L(\theta) \approx \frac{1}{N} \sum_{i=1}^N \mathbb{I} \left( d(\tilde{d}(\theta), d) \leq \epsilon \right)$$



$\epsilon$  can be adaptively reduced  
(Population Monte Carlo)

# Why is likelihood-free rejection so expensive?

1. It rejects most samples when  $\epsilon$  is small
2. It does not make assumptions about the shape of  $L(\theta)$
3. It uses only a fixed proposal distribution, not all information available
4. It aims at equal accuracy for all regions in parameter space



$$L(\theta) \approx \frac{1}{N} \sum_{i=1}^N \mathbb{I} \left( d(\tilde{d}(\theta), d) \leq \epsilon \right)$$

Proposed solution:

## BOLFI: *Bayesian Optimisation for Likelihood-Free Inference*

1. It rejects most samples when  $\epsilon$  is small

➡ Don't reject samples: learn from them!

2. It does not make assumptions about the shape of  $L(\theta)$

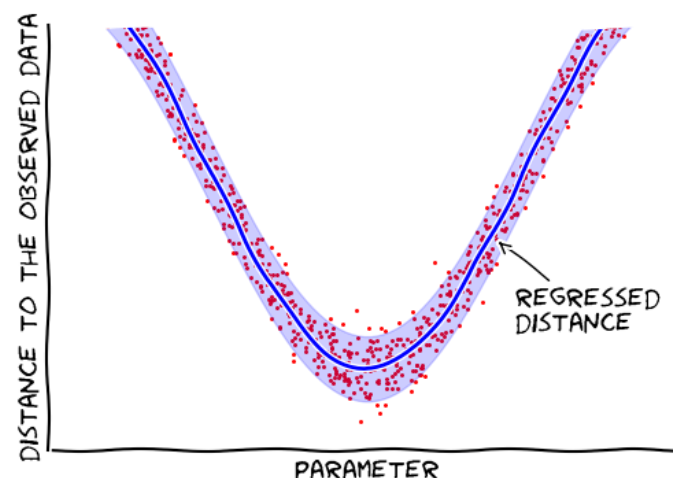
➡ Model the distances, assuming the average distance is smooth

3. It uses only a fixed proposal distribution, not all information available

➡ Use Bayes' theorem to update the proposal of new points

4. It aims at equal accuracy for all regions in parameter space

➡ Prioritize parameter regions with small distances to the observed data



Related work in cosmology:

Alsing & Wandelt 2017, arXiv:1712.00012

(data compression for ABC)

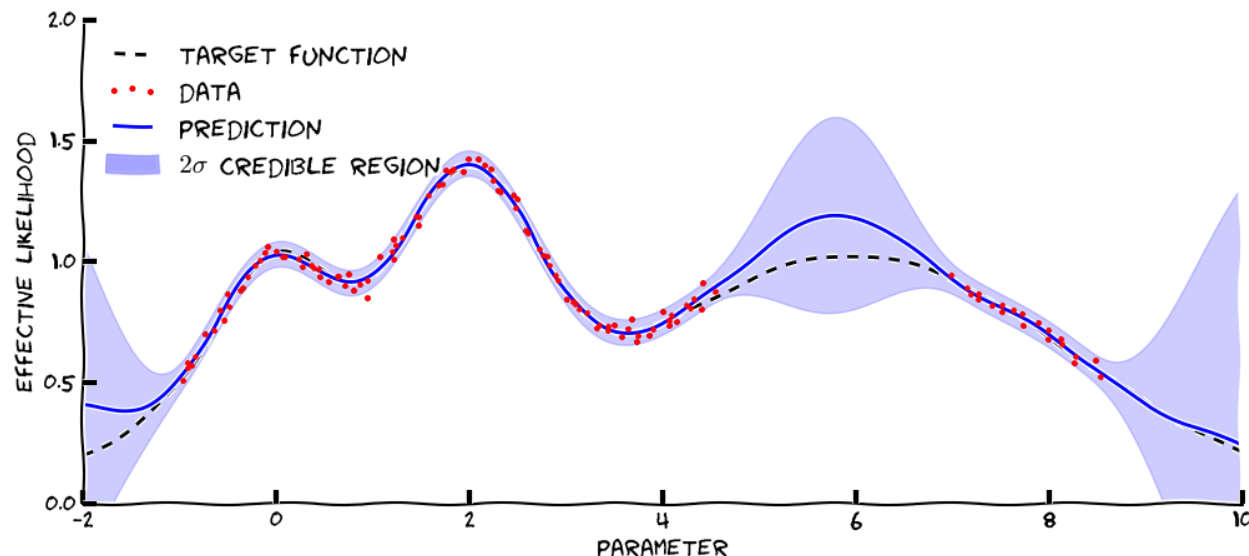
Alsing, Wandelt & Feeney 2018, arXiv:1801.01497

(density estimation for ABC – DELFI)

Enzi, Jasche & FL 2018, to be submitted

(ABC with linear expansion of the effective likelihood)

# Regressing the effective likelihood (points 1 & 2)

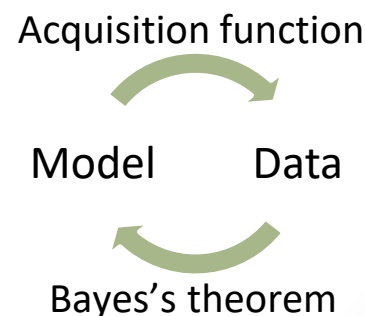


1. “It rejects most samples when  $\epsilon$  is small”
  - Keep all values  $(\theta_i, d_i)$        $d_i = d(\tilde{d}(\theta_i), d)$
2. “It does not make assumptions about the shape of  $L(\theta)$ ”
  - Model the conditional distribution of distances given this training set

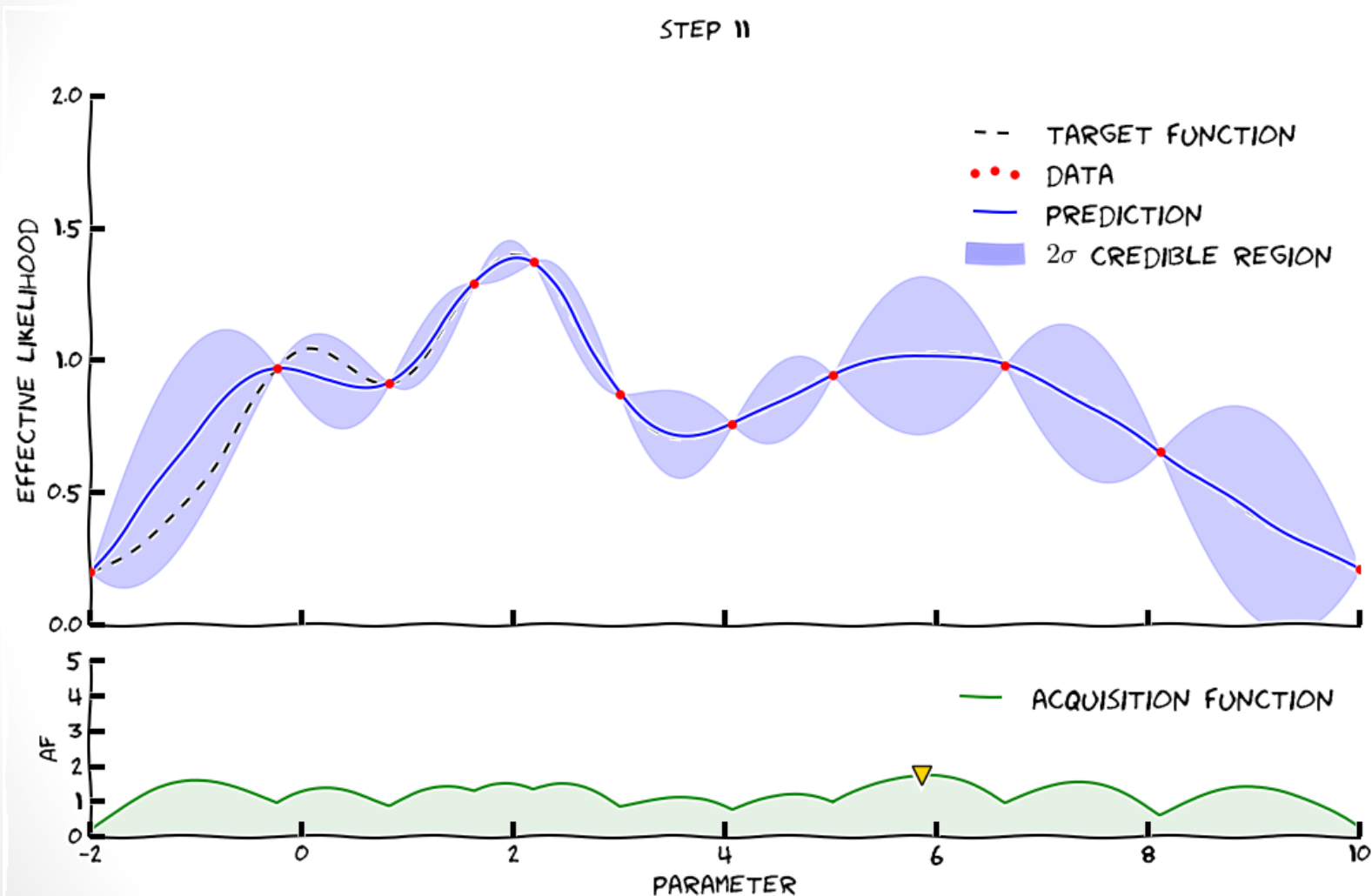


# Data acquisition (points 3 & 4)

3. “It uses only a fixed proposal distribution, not all information available”
  - Samples are obtained from sampling an **adaptively-constructed proposal distribution**, using the regressed effective likelihood
4. “It aims at equal accuracy for all regions in parameter space”
  - The **acquisition function** finds a compromise between exploration (trying to find new high-likelihood regions) & exploitation (giving priority to regions where the distance to the observed data is already known to be small)
  - **Bayesian optimisation** (decision making under uncertainty) can then be used

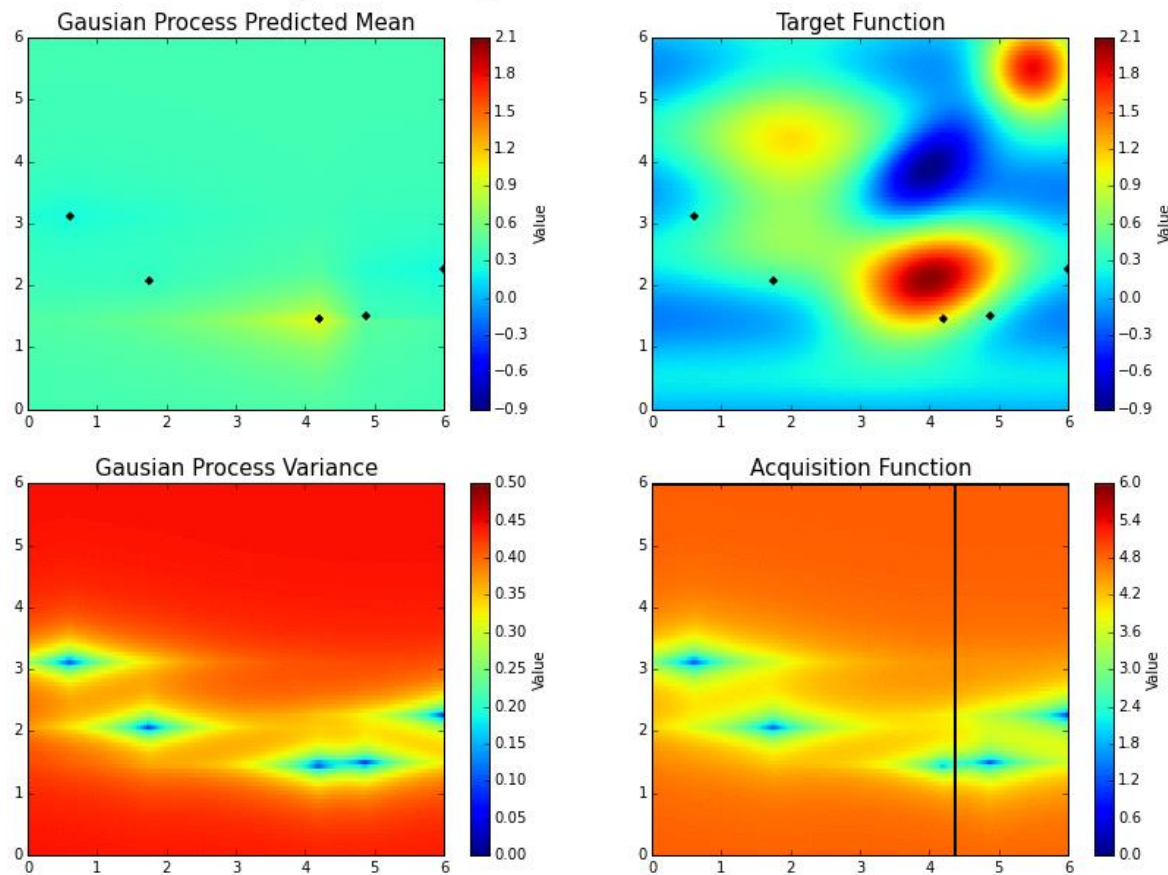


# Data acquisition



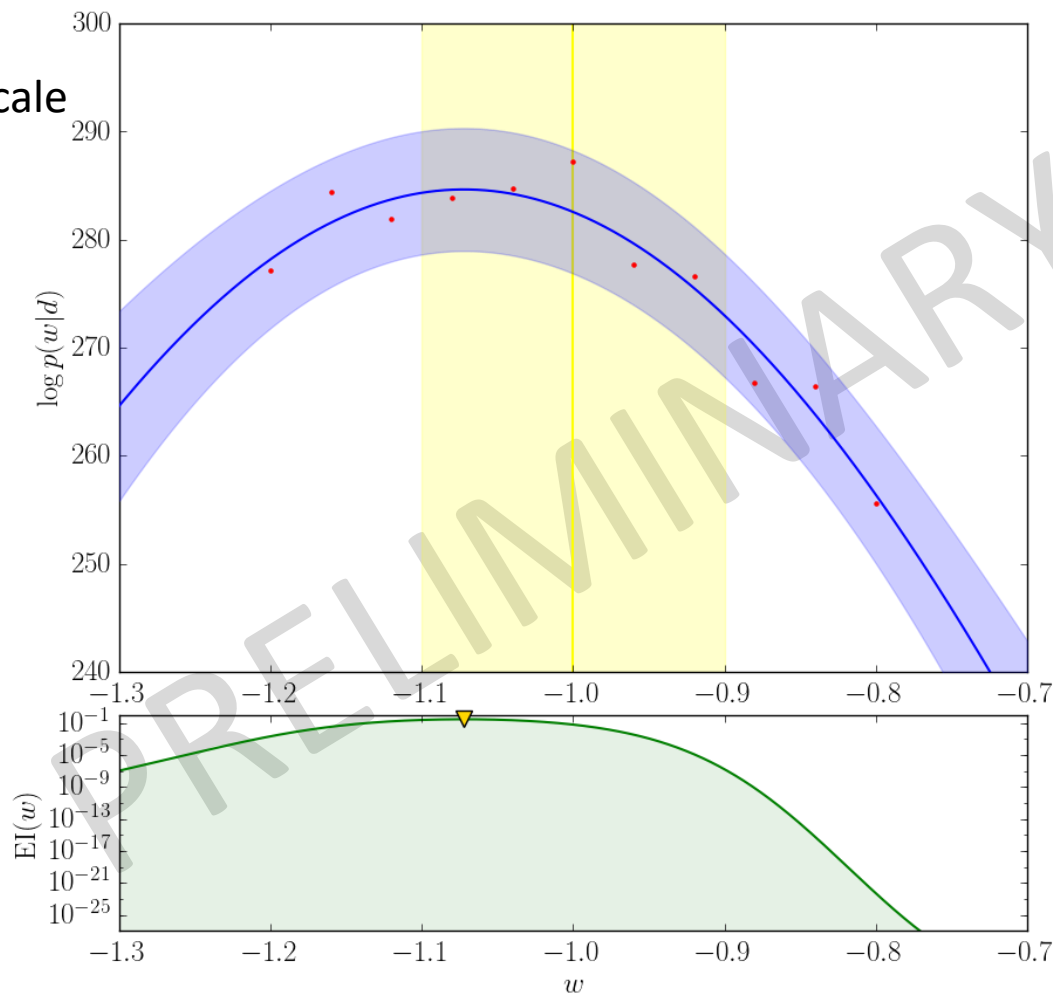
# In higher dimension...

## Bayesian Optimization in Action

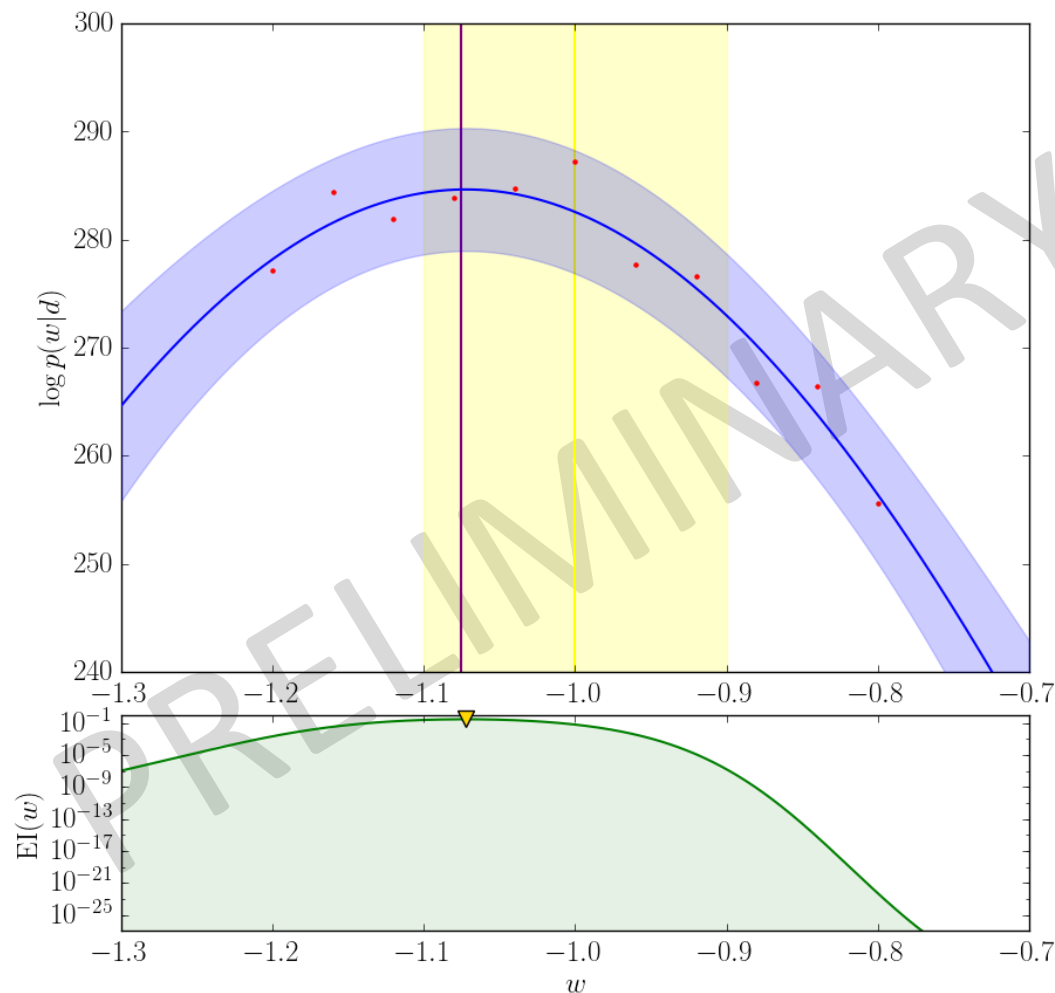


# Likelihood-free large-scale structure inference

- 1100 large-scale structure simulations using COLA
- $\approx 10^7$  hidden variables



# Likelihood-free large-scale structure inference



This proof-of-concept has been performed  
completely blindly.



# Summary

## Bayesian large-scale structure inference



- A likelihood-based method for principled analysis of galaxy surveys:  
**Hamiltonian Monte Carlo (BORG)**
  - Simultaneous analysis of the morphology and formation history of the large-scale structure.
  - Characterization of the dynamic cosmic web underlying galaxies.
- A likelihood-free method for models where the likelihood is intractable but simulating is possible:  
**Regression of the distance + Bayesian optimisation (BOLFI)**
  - Number of required simulations reduced by several orders of magnitude.
  - The approach will allow to **ask targeted questions to cosmological data**, including all relevant physical and observational effects.